Ethanone, 1-(3-hydroxyphenyl)-

121-71-1 | DTXSID5059533

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 47.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.35e-01

Confidence level: 7.76e-01

Nearest Neighbors from the Training Set

Image not found
Methyl benzoate
Measured: 126
Predicted: 58.6

Image not found
4-Methylbenzoic acid
Measured: 58.9
Predicted: 51.9

Image not found
Acetanilide
Measured: 26.9
Predicted: 40.2

Image not found
Phenylacetic acid
Measured: 28.2
Predicted: 43.1

Image not found
N-(3-Fluorophenyl)acetamide
Measured: 37.2
Predicted: 43.8